

Topological susceptibility in two-flavor lattice QCD with exact chiral symmetry

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Abstract

We determine the topological susceptibility χ_t in two-flavor QCD using the lattice simulations at a fixed topological sector. The topological charge density is unambiguously defined on the lattice using the overlap-Dirac operator which possesses exact chiral symmetry. Simulations are performed on a $16^3 \times 32$ lattice at lattice spacing ~ 0.12 fm at six sea quark masses m_q ranging in $m_s/6 - m_s$ with m_s the physical strange quark mass. The χ_t is extracted from the constant behavior of the time-correlation of flavor-singlet pseudo-scalar meson two-point function at large distances, which arises from the finite size effect due to the fixed topology. In the small m_q regime, our result of χ_t is proportional to m_q as expected from chiral effective theory. Using the formula $\chi_t = m_q \Sigma / N_f$ by Leutwyler-Smilga, we obtain the chiral condensate in $N_f = 2$ QCD as $\Sigma^{\overline{\text{MS}}}(2 \text{ GeV}) = [252(5)(10) \text{ MeV}]^3$, in good agreement with our previous result obtained in the ϵ -regime.

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The vacuum of Quantum Chromodynamics (QCD) has a non-trivial topological structure. The cluster property and the gauge invariance require that the ground state must be the θ vacuum, a superposition of gauge configurations in different topological sectors. The topological structure is also essential for the $U(1)$ problem, *i.e.* the flavor singlet pseudo-scalar meson *knows* the presence of non-trivial topological charge in the QCD vacuum. Therefore, the topological excitations, such as the instantons, played a central role in the past attempts to understand the QCD vacuum since the early years of QCD.

The topological charge fluctuations are characterized by the topological susceptibility χ_t , defined as $\chi_t \equiv \langle Q^2 \rangle / \Omega$ through the topological charge Q in a given volume Ω . Since the topological excitations do not occur in the perturbation theory, theoretical calculation of χ_t from the QCD Lagrangian necessarily involves non-perturbative methods, such as the numerical simulation of lattice QCD.

Lattice calculation of χ_t has become reasonably precise in the quenched approximation [1, 2], which is however not realistic as the quark loop effects are discarded. On the other hand, despite much effort, more realistic calculation without quenching remains a challenging problem. For instance, in full QCD, χ_t is expected to linearly depend on the quark mass and to vanish in the chiral limit. Even such a basic property has not been clearly reproduced in the previous lattice calculations (for a recent study, see, e.g., [3]).

The main difficulties are the following. (i) Definition of the topological charge density using the gauge links (discretization of $(1/32\pi^2)\epsilon_{\mu\nu\rho\sigma}\text{tr}(F_{\mu\nu}F_{\rho\sigma})$) causes bad ultraviolet divergences, while the cooling methods devised to tame the short distance fluctuations introduce sizable systematic uncertainties. (ii) Unquenched simulations with Wilson/staggered fermion do not respect correct chiral or flavor symmetry at finite lattice spacing, and the definition of the topological charge through the Atiyah-Singer index theorem is ambiguous. (iii) With the molecular-dynamics-type algorithms, which are based on a continuous evolution of the gauge links, the system is trapped in a fixed topological sector as the continuum limit is approached. Therefore, a proper sampling of different topological sectors cannot be achieved. Approaching the chiral limit (or the physical up and down quark masses) also makes the tunneling of topological charge a rare event, because of the suppression of the fermion determinant for large topological charges.

During the last decade, (i) and (ii) have been solved by the realization of exact chiral symmetry on the lattice, with which the topological charge is uniquely defined at any finite

lattice spacing by counting the number of fermionic zero-modes. (For recent studies respecting the exact chiral symmetry, we refer [4, 5].) However, (iii) remains insurmountable, since the correct sampling of topology becomes increasingly more difficult towards realistic simulation with lighter quarks and finer lattices. A plausible solution is to perform QCD simulations in a fixed topological sector and to extract χ_t from local topological fluctuations. In [6] (see also [7]), a general formula to transcribe any observable measured at a fixed topological charge to its value in the θ vacuum is derived. As an application, a new method to calculate χ_t is also proposed.

In this paper, we use this method to precisely calculate χ_t in two-flavor lattice QCD with exact chiral symmetry. The results are compared with the prediction from chiral perturbation theory (χ PT) [8]

$$\chi_t = \frac{m_q \Sigma}{N_f} + \mathcal{O}(m_q^2), \quad (1)$$

for N_f flavors of sea quarks with mass m_q . The chiral condensate Σ can be determined independently, *e.g.* from the low-lying eigenvalues of the Dirac operator [9, 10]. Therefore, the comparison provides a critical test of the lattice approach to study the QCD vacuum in the chiral regime.

A two-point function of the topological charge density $\rho(x)$ calculated in a finite volume Ω at a given topological charge Q behaves as [6]

$$\lim_{|x| \rightarrow \infty} \langle \rho(x) \rho(0) \rangle_Q = \frac{1}{\Omega} \left(\frac{Q^2}{\Omega} - \chi_t - \frac{c_4}{2\chi_t \Omega} \right) + \mathcal{O}(\Omega^{-3}) \quad (2)$$

where $c_4 = -(\langle Q^4 \rangle - 3\langle Q^2 \rangle^2)/\Omega$. The expectation value $\langle \cdots \rangle_Q$ denotes an average in a given topological sector Q . The correlation does not vanish even for large separations, because of the violation of the clustering property at fixed topological charge. We emphasize that the derivation of (2) relies only on modest assumptions such as $\langle Q^2 \rangle \gg 1$ and $Q \ll \langle Q^2 \rangle$, which are the conditions to apply the saddle point expansion in the Fourier transform from a fixed θ to a fixed Q . Except for these conditions, the formula is model independent.

We consider, in particular, two spatial sub-volumes at t_1 and t_2 , for which the correlator is defined as

$$C(t_1 - t_2) \equiv \langle Q(t_1) Q(t_2) \rangle = \sum_{\vec{x}_1, \vec{x}_2} \langle \rho(x_1) \rho(x_2) \rangle, \quad (3)$$

where the summations run over the spatial sites \vec{x}_1 and \vec{x}_2 at t_1 and t_2 , respectively. Its plateau at large $|t_1 - t_2|$ can be used to extract χ_t , provided that $|c_4| \ll 2\chi_t^2 \Omega$.

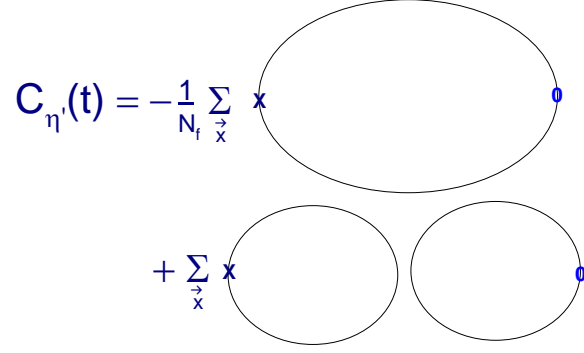


FIG. 1: A schematic diagram for the time-correlation function of the flavor singlet operator $P^0(x)$. Each solid line denotes the valence quark propagator.

In order to preserve the exact chiral symmetry, which is essential for the definition of the topological charge, we employ the overlap-Dirac operator [12, 13]

$$D(m_q) = \left(m_0 + \frac{m_q}{2}\right) + \left(m_0 - \frac{m_q}{2}\right) \gamma_5 \text{sgn}[H_W(-m_0)] \quad (4)$$

with mass m_q . The kernel operator $H_W(-m_0)$ is the conventional Wilson-Dirac operator with a large negative mass term $-m_0$.

In place of the topological charge density $\rho(x)$ (and $\rho(0)$) in (2), we use $m_q P^0(x)$ (and $m_q P^0(0)$), that were shown to give the same asymptotic constant as (2) [6] (the original suggestion is in [11]), where $P^0(x)$ is the flavor singlet pseudo-scalar density $P^0(x) \equiv \frac{1}{N_f} \sum_{f=1}^{N_f} \bar{\psi}^f(x) \gamma_5 [1 - aD(0)/(2m_0)] \psi^f(x)$. The correlator $C_{\eta'}(t) \equiv \sum_{\vec{x}} \langle P^0(x) P^0(0) \rangle$ contains a connected and a disconnected diagram as shown in Fig. 1. If we pick the disconnected piece and identify a “topological charge density”, it can be written as $\rho_1(x) = m_q \text{tr}[\gamma_5 (D_c + m_q)_{x,x}^{-1}]$, where D_c is a chirally-symmetric ($\gamma_5 D_c + D_c \gamma_5 = 0$) nonlocal operator, relating to $D(0)$ by $D_c = [1 - aD(0)/(2m_0)]^{-1} D(0)$ [14]. Integrated over the entire lattice volume, $\rho_1(x)$ reduces to the number of fermionic zero-modes, and thus has the necessary property for the topological charge density. This implies that the correlator $\langle \rho_1(x) \rho_1(0) \rangle$ has the same asymptotic constant as (2). However, the correlator $\langle m_q P^0(x) m_q P^0(0) \rangle$ approaches the constant with the rate governed by the η' mass, $e^{-m_{\eta'}|x|}$, which is much faster than $e^{-m_\pi|x|}$ appearing in $\langle \rho_1(x) \rho_1(0) \rangle$.

Simulations are carried out for two-flavor ($N_f = 2$) QCD on a $16^3 \times 32$ lattice at a lattice spacing ~ 0.12 fm. For the gluon part, the Iwasaki action is used at $\beta = 2.30$ together with unphysical Wilson fermions and associated twisted-mass ghosts [15]. The unphysical degrees

of freedom generate a factor $\det[H_W^2(-m_0)/(H_W^2(-m_0) + \mu^2)]$ in the partition function (we take $m_0 = 1.6$ and $\mu = 0.2$) that suppresses the near-zero eigenvalue of $H_W(-m_0)$ and thus makes the numerical operation with the overlap operator (4) substantially faster. Furthermore, since the exact zero eigenvalue is forbidden, the global topological charge is preserved during the molecular dynamics evolution of the gauge field. Our main runs are performed at $Q = 0$, while $Q = -2$ and -4 configurations are also generated at one sea quark mass in order to check the consistency as described below. Ergodicity within a given global topological charge is satisfied if the configuration space of that topological sector forms a connected manifold. This is indeed the case in the continuum SU(3) gauge theory on a four-dimensional torus, and therefore is probably also true at small lattice spacing adopted in this work.

We use the Hybrid Monte Carlo algorithm [16] with the mass preconditioning [17]. The fermion masses for the preconditioner were chosen to be 0.4 for heavier sea quark masses and 0.2 for the two lightest ones (see later). We exploit the rational approximation *a la* Zolotarev for the sign function in (4) after projecting out low-lying eigenmodes of $H_W(-m_0)$. With the number of poles in the rational function to be 8–10, the accuracy of $O(10^{-(7-8)})$ is achieved for the sign function. The simulations have been done in two phases for each sea quark mass. In the first phase the nested conjugate gradient (CG) is used to invert the overlap operator (4) (see [18, 19] for details). On the other hand, in the second phase we use the five-dimensional implementation of the overlap solver without the low-mode projection. The target accuracy of $O(10^{-(7-8)})$ is maintained by adding an additional Metropolis step calculated with the nested CG [20].

For the sea quark mass m_q we take six values: 0.015, 0.025, 0.035, 0.050, 0.070, and 0.100 that cover the mass range $m_s/6 - m_s$ with m_s the physical strange quark mass. After discarding 500 trajectories for thermalization, we accumulate 10,000 trajectories in total for each sea quark mass. In the calculation of χ_t , we take one configuration every 20 trajectories, thus we have 500 configurations for each m_q . For each configuration, 50 conjugate pairs of lowest-lying eigenmodes of the overlap-Dirac operator $D(0)$ are calculated using the implicitly restarted Lanczos algorithm and stored for the later use. In these calculations, the better accuracy of $O(10^{-12})$ is enforced for the sign function by increasing the number of poles in the rational approximation.

For the connected diagram (see Fig. 1), the pion correlator is computed using the con-

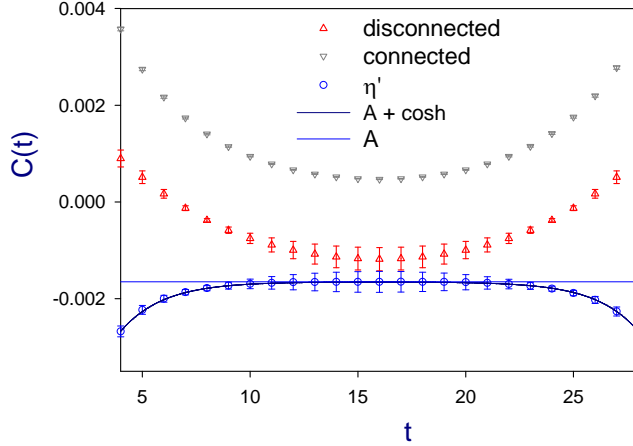


FIG. 2: Time-correlation function of the flavor singlet η' (circles) and its connected (triangle down) and disconnected (triangle up) contributions. Data at $m_q = 0.025$ are shown.

jugate gradient algorithm with a low-mode preconditioning. Low-modes are also used for averaging over source points [21], which significantly improves the statistical signal. For the disconnected diagram, the quark propagator is represented by the eigenmode decomposition and approximated by the 50 conjugate pairs of the low-lying eigenmodes. The quark propagator is then obtained for any source point without extra computational cost, and the disconnected loops can be calculated with an average over the source point. The truncation is motivated by the expectation that the long distance correlation is dominated by the low-lying fermion modes; its validity has to be checked numerically (see below).

In Fig. 2, we plot $C_{\eta'}(t)$ together with those of connected and disconnected parts for $m_q = 0.025$. The curve is the fit to the function $A + B(e^{-Mt} + e^{-M(T-t)})$ with data for $C_{\eta'}(t)$ in the range $t \in [4, 28]$. The horizontal line is the fitted constant A , and the curvature of the data points represents the contamination by the flavor-singlet state η' , that rapidly decays due to its heavy mass. Assuming $|c_4| \ll 2\chi_t^2\Omega$, we obtain $a^4\chi_t = 3.40(27) \times 10^{-5}$ at $m_q = 0.025$. The error is estimated using the jackknife method with bin size of 20 configurations, with which the statistical error saturates.

Since the disconnected diagram is computed with only 50 pairs of low-lying eigenmodes, we have to check whether they suffice to saturate $C_{\eta'}(t)$. For the time range $[4, 28]$ used for fitting, as the number of eigenmodes is increased from 10 to 30, the change of correlator $|\delta C_{\eta'}|/C_{\eta'}$ is $\sim 3\%$, while from 30 to 50, it is only $\sim 0.3\%$, which is less than 8% of the statistical error. Thus $C_{\eta'}$ is well saturated with 50 eigenmodes. This also holds for all six

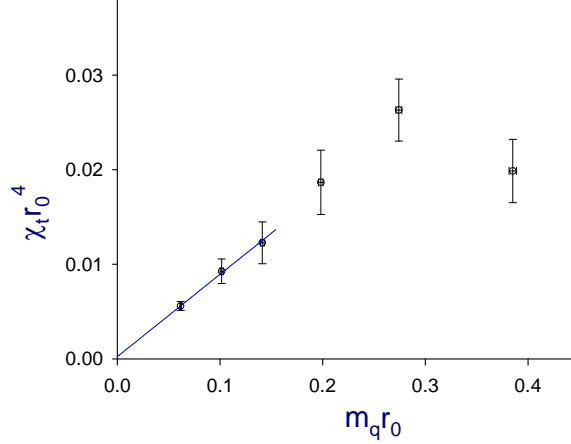


FIG. 3: Topological susceptibility $\chi_t r_0^4$ versus sea quark mass $m_q r_0$.

sea quark masses.

In Fig. 3, we plot the topological susceptibility $\chi_t r_0^4$ as a function of the sea quark mass $m_q r_0$, where r_0 is the Sommer scale extracted from the static quark potential. We also present our data in Table I, together with the lattice spacing a determined from the static quark potential with the input $r_0 = 0.49$ fm [19], and the pseudoscalar mass $m_\pi r_0$ [22]. The statistical precision is good enough to find a clear dependence on the sea quark mass. For the smallest three quark masses, 0.015, 0.025, and 0.035, the data are well fitted by a linear function $F + Gm$ with the intercept $F = 0.2(3) \times 10^{-3}$ and the slope $G = 0.087(4)$. Evidently, the intercept is consistent with zero, in agreement with the χ PT expectation (1). Equating the slope to $r_0^3 \Sigma / N_f$, we obtain $r_0^3 \Sigma = 0.174(8)$.

In order to convert Σ to that in the $\overline{\text{MS}}$ scheme, we calculate the renormalization factor $Z_m^{\overline{\text{MS}}}(2 \text{ GeV})$ using the non-perturbative renormalization technique through the RI/MOM scheme [23]. Our result is $Z_m^{\overline{\text{MS}}}(2 \text{ GeV}) = 0.742(12)$ [22]. With $a^{-1} = 1670(20)(20)$ MeV determined with $r_0 = 0.49$ fm [18, 19], the value of Σ is transcribed to $\Sigma^{\overline{\text{MS}}}(2 \text{ GeV}) = [252(5)(10) \text{ MeV}]^3$, which is in good agreement with our previous result $[251(7)(11) \text{ MeV}]^3$ [9, 10] obtained in the ϵ -regime from the low-lying eigenvalues. The errors represent a combined statistical error (a^{-1} and $Z_m^{\overline{\text{MS}}}$) and the systematic error estimated from the higher order effects (*e.g.*, c_4 term), respectively. Since the calculation is done at a single lattice spacing, the discretization error cannot be quantified reliably, but we do not expect much larger error because our lattice action is free from $O(a)$ discretization effects.

In principle, χ_t in (2) is universal for any topological sector. We check the universality of

TABLE I: The topological susceptibility $\chi_t r_0^4$ versus the quark mass $m_q r_0$ obtained in this work. The lattice spacing a for each quark mass is determined from the static quark potential with the input $r_0 = 0.49$ fm [19].

$m_q a$	$a[\text{fm}]$	$m_\pi r_0$	$m_q r_0$	$\chi_t r_0^4$	$\chi_t \Omega$
0.015	0.1194(15)	0.7096(102)	0.0616(8)	$5.59(47) \times 10^{-3}$	2.582(88)
0.025	0.1206(18)	0.8935(137)	0.1016(15)	$9.26(1.29) \times 10^{-3}$	4.454(356)
0.035	0.1215(15)	1.053(13)	0.1412(17)	0.0123(22)	6.078(794)
0.050	0.1236(14)	1.238(14)	0.1982(22)	0.0187(34)	9.900(1.354)
0.070	0.1251(13)	1.456(15)	0.2742(28)	0.0263(33)	14.65(1.21)
0.100	0.1272(12)	1.734(17)	0.3852(36)	0.0199(33)	11.82(1.55)

χ_t as follows. At sea quark mass $m_q = 0.050$, we generate 250 configurations with $Q = -2$ and -4 respectively in addition to the main run at $Q = 0$. Then we extract χ_t from the time-correlation function of η' , similar to the $Q = 0$ case. Our results for $a^4 \chi_t$ are: $\{7.4(1.3), 6.4(2.1), 5.9(1.8)\} \times 10^{-5}$ for $Q = \{0, -2, -4\}$ respectively. Evidently, χ_t extracted from different topological sectors are consistent with each other within the statistical error.

Finally, we discuss on the neglected terms in (2). The leading correction comes from the $|c_4| \ll 2\chi_t^2 \Omega$ term. With the formulas derived in [6], we can obtain an estimate of the upper bound of $|c_4|/(2\chi_t^2 \Omega)$ by measuring the two-point correlator $\langle \rho_1(x_1) \rho_1(x_2) \rangle$ and the four-point correlator $\langle \rho_1(x_1) \rho_1(x_2) \rho_1(x_3) \rho_1(x_4) \rangle$. Our preliminary result is $|c_4|/(2\chi_t^2 \Omega) < 0.1$, for all six sea quark masses. Details of this calculation will be presented elsewhere. We note that this upper bound is also consistent with the ratio $|c_4|/\chi_t \simeq 0.3$ obtained in the quenched approximation [24, 25].

In this letter, we have determined the topological susceptibility χ_t in two-flavor QCD from a lattice calculation of two-point correlators at a fixed global topological charge. The expected sea quark mass dependence of χ_t from χ PT is clearly observed with the good statistical precision we achieved, in contrast to the previous unquenched lattice calculations. Our result indicates that the topologically non-trivial excitations (*e.g.*, instanton and anti-instanton pairs) are in fact locally active in the QCD vacuum, even when the global topological charge is kept fixed. The information of these topological excitations is carried

by low-lying fermion eigenmodes if the exact chiral symmetry is respected on the lattice. This work demonstrates that Monte Carlo simulation of lattice QCD with fixed topology is a viable approach, to be pursued when the topology change hardly occurs near the continuum limit even with chirally non-symmetric lattice fermions. The artifacts due to the fixed topology in a finite volume can be removed to obtain the physics results in the θ vacuum, provided that χ_t has been determined in the first place [6, 7] as has been done in this work.

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